Segmented regression in thermo-physics modeling

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Traditionally in applied thermo-physics the temperature dependence of the heat capacity is described by polynomials in temperature (from 298K to the melting point) [1], with adjustable parameters fitted to experimental data. The effort to extend that description to low temperature demands more physical modeling which takes into account the recently available theoretical data.

The more physical approach requires the modeling of several contributions (e.g. electronic, vibrational, etc.) that appear in different temperature ranges [2].

In this work we propose the development of statistical segmented models, that can be used as a support tool for CALPHAD[a] modeling [3] and we implement them in *R* [4, 5]. Several segmented regression functions were considered and analyzed, with the corresponding confidence intervals being calculated using the bootstrap method. Moreover we validate the consistency of underlying fitting results, by calculating other physical properties of interest, such as the enthalpy, that can be derived directly from the heat capacity of the studied material.

An overview of available functionalities in the *R* software package for segmented regression [6, 7] will be discussed in solving the nonlinear equations arising from complex model that has to be applied.

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[a] CALPHAD = CALculation of Phase Diagramm